

COPY 2  
ACCN: 223972



**RAL Report**  
RAL-94-087

# The PRSPLOT6 Manual

COMP, HEP

**M Hagen**

August 1994

**Rutherford Appleton Laboratory** Chilton DIDCOT Oxfordshire OX11 0QX

**DRAL is part of the Engineering and Physical Sciences Research Council**

The Engineering and Physical Sciences Research Council does not accept any responsibility for loss or damage arising from the use of information contained in any of its reports or in any communication about its tests or investigations

# The PRSPLOT6 Manual

Mark Hagen

Department of Physics  
Keele University  
Keele, Staffs. ST5 5BG, U.K.

And

ISIS Science Division  
Rutherford Appleton Laboratory  
Chilton, Didcot  
Oxon. OX11 0QX, U.K.

July 29, 1994

## Contents

<b>1</b>	<b>Introduction</b>	<b>3</b>
<b>2</b>	<b>Load — Input data from a file</b>	<b>4</b>
<b>3</b>	<b>Draw — Draw initial plot of data, qualifiers /M /L /E /I /B /S /C</b>	<b>6</b>
<b>4</b>	<b>Plot — Overplot data, qualifiers /M /L /E /I /B /S /C /A /X /Y</b>	<b>6</b>
<b>5</b>	<b>Alter — parameters for text/axes, data points/lines, contour levels</b>	<b>7</b>
5.1	Text/axes parameters — qualifiers /H /F /N /X /Y . . . . .	7
5.1.1	C for Characters . . . . .	7
5.1.2	T for Tick Marks . . . . .	7
5.1.3	V for Values . . . . .	7
5.2	Data symbols and linetypes . . . . .	7
5.2.1	M for Markers — qualifiers /H . . . . .	7
5.2.2	L for Lines . . . . .	8
5.2.3	S for Smoothness . . . . .	8
5.3	I for contour level parameters — qualifiers /H /N /P . . . . .	8
5.3.1	/H for contour level heights . . . . .	8
5.3.2	/N to change normalisation parameters . . . . .	8
5.3.3	/P for miscellaneous parameters . . . . .	8
<b>6</b>	<b>X — Extract data from intensity map, qualifiers /N /D /E /Q /P</b>	<b>9</b>
<b>7</b>	<b>O — Output workspace or normalisation parameters to a file</b>	<b>10</b>
<b>8</b>	<b>S — Save plot in postscript output file</b>	<b>10</b>
<b>9</b>	<b>J — Run system command or create a subprocess</b>	<b>10</b>
<b>10</b>	<b>Menu — Change size and orientation of plot</b>	<b>10</b>
<b>11</b>	<b>Title — Change axis titles for a workspace</b>	<b>10</b>
<b>12</b>	<b>Reset — Reset default parameters</b>	<b>11</b>
<b>13</b>	<b>Special Characters in Titles</b>	<b>11</b>
<b>14</b>	<b>Error reporting</b>	<b>11</b>

## 1 Introduction

The PRSPLOT6 program can be used to plot data from PRISMA experiments in the form of either extended zone dispersion relations or contour maps and can be used to extract ( and plot ) data from contour maps. The program is available on the ISISE and ISVS5 VAX VMS computers at RAL and on the potter SUN SPARCcenter (UNIX) computer at Keele. It uses plotting subroutines from the UNIRAS library. For most of the program the code is identical on both the VAX and UNIX systems, however there is some system dependent code, to do with renaming files, creating sub-processes and the inability of UNIRAS to work properly on a terminal emulating a TEK 4010 on a UNIX system. This system dependent code is all contained in the file `j4jump.for`. On the VAX systems the code is kept in the directory `user$disk:[knh.prisma.colour]` and can be linked using the `colink.com` file in this directory. On the potter computer the code is in the directory `/users/ph/pha70/caco3` and can be compiled and linked by using the executable file `plrs`.

The program is designed to let the user interactively create a plot at the terminal from data read in from a file(s) and then to get a postscript or colour postscript (colourview at Keele) output file. It consists of 11 commands and their qualifiers and parameters. The commands are **D**raw, **P**lot, **L**oad, **A**lter, **S** to create a laser plotter file, **M**enu to alter the size and proportion of the plot, **T**itle to alter the text annotation, **R**eset to reset all parameters changed by the alter command, **J**ump to create a subprocess or run a system command, **X** to extract data from a contour map and **O**utput data in a workspace to a file. The program prompts with an `>` symbol. The structure of a command line consists of a one letter symbol, specifying the command, its qualifiers (if any) which are separated from the command and each other by `/`'s, a space between the command/qualifiers and the parameters for the command, which are in turn separated by spaces. The command symbols, qualifiers and workspace symbols may be either upper or lowercase characters. A description of the commands and their qualifiers and parameters is given in the following sections.

The program can be run on (1) terminals emulating a vt100 alpha and tektronix 4010 graphics setup (eg. Pericom or Falco), (2) a colour X11 terminal (or workstation, eg. Vaxstation 3100 or 4000 or colour Sun) or (3) a P.C. emulating a tektronix 4200 series colour terminal (eg. the TEEMTALK or EMUTEK emulators). Obviously option (1) doesn't allow colour plots to be made. Option (2) requires that (if necessary) the DISPLAY variable has been set-up correctly for the output window. On starting the program, which is done by typing `prspplot6` (on both UNIX and VAX systems) the user will be prompted to choose one of the above options for the terminal type. Following this the user is prompted for the type of hardcopy output file. Option (1) is a simple black and white postscript file, option (2) is a colour postscript file and option (3) is a file for the Calcomp Colourview plotter at Keele.

## 2 Load — Input data from a file

The load command (L) is used to get data into the prsplot6 program ready for plotting. It has the structure

**L W<sub>n</sub> filename**

where W<sub>n</sub> is a workspace from W1 to W120 and filename is the name of the file containing the data to be loaded. If the file is not in the current working directory then the filename should include the pathname to find the file. Note this doesn't work on the UNIX systems since they use /'s to delimit directory names and the program gets confused with /'s for qualifiers. Issuing the load command above leads to a menu which requests the type of file to be loaded. There are 6 data file options which are as follows.

### (1) E vs Q trajectories and (2) Data points

These two options take very similar input. The first will load a workspace with the E vs Q values for a PRISMA measuring trajectory ready for plotting. The second will take a file of data points (eg. phonon peak energies), in the format of 2 or 3 columns, column 1 is detector number, column 2 is position in energy transfer and column 3 (which is optional) is the error in the value of column 2 and plot these data points on an E vs Q diagram following the PRISMA measuring trajectory. Note that error bars will be correctly plotted at an angle (ie. following the trajectory). The filename in the load command given above should be the name of a file containing the OLDNOTES.TXT data appropriate to the plot. If this name is omitted then the default name OLDNOTES.TXT will be used, although you will be prompted to check this (even in fact if you entered another name you will be prompted). You will also be prompted for the choice of x-axis variable (H, K or L) in both cases. However for option (1) you will then be prompted for which detector number you wish to load the trajectory for and for option (2) you will be prompted for the name of the file which contains the data points. For option (2) you will then be prompted to say whether the file contains error bars or not (ie. whether there is a column 3 in the format described above).

### (3) Dispersion relations

This option loads a file which contains two columns of numbers, column 1 is the x-values and column 2 the y-values. The name refers to the fact that it could be a theoretical dispersion relation to be plotted for comparison with the data points. Alternatively it could just be a line to be drawn on the data. The file name in the load command must be supplied on the load line. The structure of the file should be as follows. The first line is a line of text (max 80 characters), the second line is the number of x-y points contained in the file (integer input). The rest of the file should be two columns of x and y values describing the "dispersion relation".

### (4) Straight lines

This option does not need (and should not have) a file name on the load command line. It simply allows a straight line to be loaded into a workspace for plotting on the figure. The user will be prompted for two end points on the straight line. The workspace will then be filled with 201 equally spaced points on a straight line between these two end points.

(5) Intensity map (inelastic) and (6) Intensity map (crit. scatt.)

These two options allow intensity maps to be loaded for plotting colour contour plots. There is a slight difference in the structure of the two types of file, the inelastic map having been created with the CC option and the elastic (or critical scattering as it is otherwise known) with either the VCRS option in GENIE. However the load command line is the same in each case and is as given above, with the filename being the name of the file containing the intensity map. Note only one intensity map can be loaded at any one time. The intensity map will contain data from a whole series of spectra (possibly different detectors or different steps in a scan). Each spectra is stored separately in a different workspace. Thus the workspace number entered in the load command line is the first workspace to be used and subsequent spectra will be stored in subsequent workspaces. For example if W1 is provided in the load line and the file contains 32 spectra then workspaces 1 to 32 will be loaded with data.

After the spectra have been loaded the user will be prompted for the name of a normalisation file, this is optional and entering no file name is allowed. However if the user wishes to modify the data set then the normalisation file allows the height of the data to be scaled and a background subtracted. The format of the file is a series of normalisation data sets, one for each run number included in the intensity map. Each normalisation data set has the following format. The first line should be the run number to which the normalisation parameters apply and the following 16 lines (and there must be 16 lines, any detectors not used must still be supplied values, albeit dummy values) are in the form, detector number, scale factor and background. The data in the intensity map is then rescaled at plotting time according to the formula

$$\text{modified data} = \text{scale factor} \times (\text{unmodified data} - \text{background})$$

Note: These normalisation values can be altered at a later stage if necessary (see section on A/N I).

Note: If the critical scattering data was normalised in VCRS with a vanadium run then no normalisation file will be needed.

The user is then prompted for the choice of x-axis variable in the plot (H, K or L). This applies to both inelastic (which will be an E vs Q plot) and elastic intensity maps. The elastic intensity map option then prompts for the choice of y-axis variable (H, K or L) and then for the angle between these two axes (the default option is 90 degrees). This latter possibility is for plotting hexagonal or other non-orthogonal co-ordinates. The choice of x-axis co-ordinate is always plotted as the x-axis but if the angle between x and y is not 90 then the y co-ordinate is "skewed" at plot time so that the correct angle between x and y axes is obtained. Note the x co-ordinate values are plotted along the x-axis of the plot but that the co-ordinates of the skewed y-axis are plotted along the (90 degree) y-axis.

Titles

At the end of the load option, whichever option has been chosen, the user will be prompted for 3 titles, 1) for the x-axis, 2) for the y-axis and 3) for the title at the top of the plot. Note that these titles can be changed at a later stage (without having to reload the data) by using the title command T (see later section on T).

### 3 Draw — Draw initial plot of data, qualifiers /M /L /E /I /B /S /C

The draw command (**D**) is used to create the initial plot on the screen. It takes the form

**D/qualifier Wn Xmin Xmax Ymin Ymax**

where Wn is the workspace to be plotted (W1 to W120) and Xmin, Xmax, Ymin and Ymax are the (optional) plotting limits. Basically there are two types of plot, either a dispersion relation type plot, where the qualifiers /M (for marker symbols), /L (for lines) or /E (for error bars) are relevant or a colour contour/intensity map where the /I (intensity map), /B (intensity boundaries), /S (shaded colour contour levels), /C (contour level boundaries) are relevant. The /I and /B qualifiers plot the data without any interpolation. Each data point has a coloured grid cell depending on its value for /I and simply plots the boundaries between grid cells where the colour changes for /B. The /S and /C qualifiers interpolate the data to connect together contour levels. The /S qualifier plots colour shaded regions for values that lie between the boundaries of two contour levels and /C plots lines for the boundary levels.

If no qualifier is provided to D the default is to plot the data in Wn as markers assuming that it is a dispersion relation plot. Clearly this will go wrong if the workspace is part of an intensity map.

### 4 Plot — Overplot data, qualifiers /M /L /E /I /B /S /C /A /X /Y

The plot command (**P**) takes two forms. Either it allows subsequent workspaces to be plotted on a graph already started with the D command or it allows the plotting of secondary axes on the graph. For the first usage the P command takes the form

**P/qualifier Wn**

and requires a qualifier which may be /M, /L or /E for dispersion relation type plots or /I, /B, /S or /C for intensity/contour maps and a parameter Wn specifying the workspace to be plotted. It is of course possible to plot markers ( /M ), lines ( /L ) or even error bars ( /E ) on an already drawn intensity or contour plot but it is unadvisable to do this the other way around. The meaning of the various qualifiers /M, /L, /E, /I, /B, /S and /C were given in the section on the draw command.

The second usage of the plot command takes the form

**P/A/X xmin xmax or P/A/Y ymin ymax**

and will label the top/right hand side of the plot (for X/Y respectively) with a secondary axis from xmin to xmax or ymin to ymax respectively. The user will be prompted for a title for the new axis. Note that subsequent to this command the scaling of the plot co-ordinates will correspond to this new axis rather than the original.

## 5 Alter — parameters for text/axes, data points/lines, contour levels

The alter command (**A**) is used to change values (heights etc. ) for the following parameters C, T, V, M, L, S and I. The first 3 parameters C, T and V relate to the way that text/numbers are plotted on the axes of the graph, the second three parameters to the way the data is plotted and the final parameter (I) to the set of parameters which define the contour levels etc. when plotting a contour/intensity map. These parameters are described below along with the relevant qualifiers to the alter command.

### 5.1 Text/axes parameters — qualifiers /H /F /N /X /Y

#### 5.1.1 C for Characters

The parameter C refers to the characters used in plotting the names of the X-axis and Y-axis, and the title of the plot. The command **A/H C r** will change the height (and corresponding width) of the characters used to r mm from the default value of 3 mm.

#### 5.1.2 T for Tick Marks

The parameter T refers to the tick marks plotted on the X and Y axes. Major tick marks are plotted at the positions where numerical values are plotted on the X and Y axes. The length of these tick marks can be changed by the command **A/H T r** from the default value of 3 mm to a value of r mm. Intermediate (or minor) tick marks can be included between the major ones, using the commands **A/N/X T n** or **A/N/Y T m** where n and m are integers. This will include n minus 1 intermediate tick values on the X axis and m minus 1 on the Y axis, the default values for n and m are 1 (no intermediate ticks).

#### 5.1.3 V for Values

The parameter V refers to the values plotted at the major tick marks on the X and Y axes. The size of the values plotted is controlled by the command **A/H V r** where r is a real number specifying a height for these values of r mm instead of the default value of 3 mm. The format with which these values are plotted can also be controlled using the commands **A/F/X V nEm** and **A/F/Y V nEm** for the X and Y axes respectively, and where n and m are integers. The specifier nEm defines the format as follows, the values are plotted with n places after the decimal point and with an exponent value of  $10^{-m}$  plotted at the end of the axis. Note that if you get the format wrong, ie the values won't fit into the format, the program will most probably crash. The number of values (major tick marks) plotted along an axis is controlled by the commands **A/N/X V n** and **A/N/Y V m** for the x and y axes respectively where n and m are integers giving the number of values to be plotted on the axis.

## 5.2 Data symbols and linetypes

### 5.2.1 M for Markers — qualifiers /H

The parameter M refers to the marker symbols used when plotting data. The command **A M n** where n is an integer from 1 to 22 will change the marker symbol used. See page 359 of the AGL/CHARTS manual for a list of symbols. The command **A/H M r** where r is a real number changes the size of the symbol to r mm from the default size of 2 mm.

### 5.2.2 L for Lines

The type of line (solid, dot-dash, etc. ) used in the D/L or P/L commands can be changed by the command **A L n** where n is an integer. The list of UNIRAS line types is given on page 49 of the FGL/GRAPHICS manual. The default value is 0 (a solid line). If a negative value for n is supplied then a dashed line will be drawn where the dashes/spaces are of length |n| mm.

### 5.2.3 S for Smoothness

In the default mode lines will be plotted by connecting the points in the workspace with straight lines. This can be changed with the command **A S n** where n is an integer 0 or 1. The default setting corresponds to an n value of 1. If this is changed to 0 then the lines will be plotted between the data points using a cubic spline interpolation routine.

## 5.3 I for contour level parameters — qualifiers /H /N /P

### 5.3.1 /H for contour level heights

The command **A/H I** leads to a menu where the lower and upper levels for contour plotting, the number of levels and the type of level scheme (linear or logarithmic) can be chosen. When data is read in with the load command for an intensity/contour map the lower and upper levels are automatically set to the smallest and largest intensity values in the data set. The contour levels are chosen as follows. Everything with a value below the minimum level is set to one colour (the lowest in the colour table) and everything above the upper level is set to one colour (chosen to be above the other colours in the colour table). The intermediate levels are set by calculating the boundary values between these levels in steps of

$$\text{step} = (\text{upper} - \text{lower}) / \text{nos of levels}$$

and assigning a colour to the values which fall between two boundaries.

### 5.3.2 /N to change normalisation parameters

When an intensity map is read in a “normalisation” file name is requested, if provided this is a table of numbers which can be applied to the data to “normalise” it when plotting. This table can be edited to change the normalisation values by using the command **A/N I** which leads to a menu for changing the values. Note the normalisation table can be written out to a file using the **O/N** command (see section on O for output command).

### 5.3.3 /P for miscellaneous parameters

This command **A/P I** is not fully implemented at the time of going to press. It will in the future allow (a) the choice of different (other than the current UNIRAS default) colour tables, (b) to shift the contour level calculation algorithm for neighbouring time of flight paths and (c) to load a contour level table defined by the user rather than the linear/logarithmic levels defined with **A/H I**.

## 6 X — Extract data from intensity map, qualifiers /N /D /E /Q /P

The X command is used to extract a “cut” through the intensity map and put the data in a workspace. It takes the general form

```
X/qualifiers Wn { parameters }
```

where in all cases the /N qualifier (which must be last in the list of qualifiers) can be used to apply the normalisation parameters to the data before extracting. The /D, /E and /Q qualifiers all apply to an inelastic intensity map. The /D qualifier extracts data for a particular detector and run number. Its form is

```
X/D Wn run_nos detector_nos x_unit
```

where `x_unit` is H,K,L or E (the default) is the co-ordinate used for x values in the output workspace. The /E qualifier extracts a constant energy cut from the intensity map. It takes the form

```
X/E Wn E_value x_unit
```

where `x_unit` is as before. Similarly the /Q qualifier is a constant Q cut and has the form

```
X/Q Wn Q_value q_unit
```

where `Q_value` is the value at which the constant Q cut is done and `q_unit` is H, K or L, the variable to which `Q_value` applies. The x axis values in the output workspace are energy transfer.

The extraction of data from an elastic intensity map is done with the /P qualifier. It takes the form

```
X/P Wn x1 y1 x2 y2 x_unit
```

where ( `x1` , `y1` ) and ( `x2` , `y2` ) are two points on a line through the intensity map along which data is extracted, and `x_unit` is H, K or L, the co-ordinate to be used for the x values in the output workspace. Note that ( `x1` , `y1` ) and ( `x2` , `y2` ) simply define a line ( they are not necessarily the end points and don't have to lie within the intensity map ) and data will be extracted everywhere that the line passes through the intensity map.

## 7 O — Output workspace or normalisation parameters to a file

The O command can be used to write out the data in a workspace to a file. The command takes the form

**O Wn filename**

where Wn is the workspace and the filename is the that of the output file. It is also possible to write out the table of normalisation parameters to a file using the O command. This is done by

**O/N filename**

## 8 S — Save plot in postscript output file

The command to make a postscript output file is (S). There is one (optional) parameter for S and no qualifiers. The way that S works is to change the output for the program from the terminal to a file called POST on potter and POST.DAT on the Vaxes and then to go through all of the A, D and P commands entered since the last D command to create the plot. Then the file POST is “moved” on potter or renamed on the Vaxes onto the optional filename argument supplied to S. If the final output name already exists a warning is printed and the user can opt not to continue. If the file POST(.DAT) exists the user is warned about overwriting and allowed to stop. Note on the Vaxes there is no problem because a new version number is created and nothing is overwritten. Note S cannot perform any L commands so that all of the data to make the plot must be in the relevant workspaces before the S command is used.

## 9 J — Run system command or create a subprocess

It is possible to use the J command either to run a system command from within prsplot6 or to create a subprocess from which system commands can be run without stopping prsplot6. The first usage takes the form

**J “command line”**

where the command line to be run is enclosed in the quotation marks. The second usage takes the form **J/P** on the Vaxes. This creates a subprocess and runs the users login.com. To get back into prsplot6 one just logs out of the subprocess. On the UNIX systems J/P doesn't work, instead one must use control-z which suspends prsplot6. To get back into prsplot6 one then types fg.

## 10 Menu — Change size and orientation of plot

The menu command, an M with no qualifiers or parameters, allows the size (in millimetres) of the plot and its orientation to be specified. Note this applies to the output printer rather than the terminal. The plot is always the same way up on the terminal and UNIRAS will do some scaling to fit the plot on the screen. Note also that there are no checks on the size of the plot, if you specify sizes too big for the plotter page it will probably chop off part of the plot when you try to print it.

## 11 Title — Change axis titles for a workspace

The command T Wn where Wn is a workspace number eg. W1, will allow you to change the text used to annotate the relevant workspace (x and y axis labels and the title). The same menu that appeared at the end of the load operation is used.

## 12 Reset — Reset default parameters

If the alter command is used to change the heights/formats/number of values on the x and y axes or text, or change the size of the plot etc. then these parameters will remain in force when subsequent workspaces are drawn. In order to “clear” these parameters back to the default situation the reset command, an R without any qualifiers or parameters, can be issued.

## 13 Special Characters in Titles

There are special characters, Greek letters and mathematical symbols available in UNIRAS and also the ability to do superscripts and subscripts (and even backspaces !!). The Greek and mathematical symbols must be included in the titles using Hershey numbers, eg. ^2136 represents  $\kappa$ . A list of Hershey numbers is given in appendix B of the FGL/GRAPHICS manual. In order to make the following symbol a superscript or subscript in the title the user must precede it with a > or < symbol respectively. In order to backspace so as to plot the next character at the same position the \_ character is used.

## 14 Error reporting

In a program as large as prsplot6 the possibility of errors/bugs/conflicts is large. If you find such a situation then you can report it by e-mailing [knh@isis-e.rutherford.ac.uk](mailto:knh@isis-e.rutherford.ac.uk) . In order to reproduce the error and track it down you'll need to provide a complete history of what you've been doing with the program, not just the last command you typed, and of course a return e-mail address to answer any questions which may be required to generate the fault.





